Lecture 9: Correlations between Steps

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In this lecture we consider a walker making random identically distributed but not independent (correlated) steps[1]. After N steps of length $\Delta\vec{x}_i$, $i = 1, .., N$, position $\vec{X}_N$ of the walker is given by:

$$\vec{X}_N = \sum_{n=1}^{N} \Delta\vec{x}_n. \tag{1}$$

The problem is: where does the walker end up after N steps? We first digress into examples of problems approximated by random walkers making correlated steps.

1 Examples

1.1 Turbulent flow of liquid

One of the first persons to consider correlation between steps of a random walker was G. I. Taylor, when in 1921 he solved the problem of turbulent diffusion of liquid. The motion of liquid can be approximated by a series of identically distributed random steps $\Delta\vec{x}_n$, exponentially correlated in time:

$$\langle \Delta\vec{x}_n \cdot \Delta\vec{x}_{n+1} \rangle = \rho\sigma^2, \qquad \text{for all } n. \tag{2}$$

Here ρ describes tendency of the walker to move in the same direction as in the previous step; σ^2 is the variance of distribution of a single step. Later in the lecture we will see that solution of the problem gives advection (i.e. directed flow) on small time scales and diffusion at larger time scales. We will see that in this problem CLT still holds, but the diffusion coefficient D is modified:

$$\frac{D}{D_0} = \frac{1+\rho}{1-\rho}, \tag{3}$$

where $D_0 = \frac{\sigma^2}{2\tau}$ is the diffusion coefficient in absence of correlation between steps.

1.2 Transmission of electrical signals along telegraph cables

This problem was considered by Lord Rayleigh in about 1880. A short electrical (voltage) pulse fed into an end of a long cable propagates at a certain velocity and spreads out in duration due to cable defects. An applicable model involving a random walker is: a walker that almost always moves forward in one direction, but sometimes makes steps back at defect points. Lord Rayleigh considered the problem in the continuum limit and solved a generalization of the diffusion equation.

[1] We emphasize that correlation is between steps of a single walker, as opposed to a more complicated problem of correlation (interaction) between different walkers.

1.3 Financial time series

Behavior of stock prices in time can be approximated by one-dimensional random walks. It was observed that increments of the prices exhibit correlations on time scales as large as ~ 10 minutes. Existence and knowledge of such correlations could be used to predict and take advantage of short-term market behavior. Hence, time scale of such correlations can be considered as a measure of market liquidity, with shorter correlations meaning a more liquid market, where it is more difficult to take advantage of these correlations to make money.

1.4 Polymer structure

Polymers are long molecular chains. Polymers are widespread in living organisms, with examples such as proteins and DNA. Polyethylene is a synthetic polymer with (CH_2) as a basic unit. In general, the long linear molecular chain is not straight, but is folded producing a conformation. A basic question one can ask is: if the polymer consists of N blocks of a certain length, what is the distance R_N between the two ends of the polymer? Is $R_N \sim b\sqrt{N}$? $R_N \sim bN^\nu$? What is ν and the coefficient of proportionality b?

Answer to these questions requires consideration of physical constraints in a model of polymer.

1. Short-range correlation (the simplest model). In many polymers the connection between the basic blocks is made between carbon atoms. Carbon atoms have 4 valence electrons and tend to make 4 covalent bonds. Carbon-carbon bonds prefer to be at a certain angle $\theta \approx 109.471$ ($\cos\theta = 1/3$). In diamond carbon atoms form a structure with every carbon atom covalently bonded to 4 surrounding it in the 3 dimensions other carbon atoms, with angle of $\theta \approx 109.471$ ($\cos\theta = 1/3$) between the bonds. As a result, carbon atoms in diamond are firmly held in place. In polymers such as proteins and polyethylene, however, a carbon atom makes connections with only 2 of its neighboring carbon atoms, with the other two bonds connecting to unconstrained in space residues (H in polyethylene). In the resulting linear structure angle between adjacent carbon-carbon bonds (tetrahedral angle θ) tends to be at $\theta \approx 109.471^\circ$, with an unconstrained rotational degree of freedom around a carbon-carbon bond, given by dihedral angle ϕ.

This leads to a simplest model of such polymer as a random walk with correlation in the tetrahedral angle θ between the steps ($\cos\theta = 1/3$) and the dihedral angle ϕ distributed randomly. Solution of the problem gives:

$$\langle \Delta\vec{x}_{n+1} \cdot \Delta\vec{x}_n \rangle = \frac{\sigma^2}{3}, \qquad \rho = \frac{1}{3}. \tag{4}$$

These correlations are exactly of the type considered earlier in the problem of turbulent flow of liquid. In this case $\rho = 1/3$ and $\frac{D}{D_0} = \frac{1+\rho}{1-\rho} = 2$, i.e. effectively correlations (4) lead to bigger spread in dimensions of the polymer, with CLT scaling $\langle \vec{X}_N^2 \rangle \sim N$ preserved.

2. Self avoidance (a more complicated constraint). This constraint requires non-intersection of the polymer with itself. Intuitively it can be easily understood that this constraint is less important in higher dimensions, since the higher the dimension, the less is the chance that a polymer will try to cross itself.

It turns out that R_N scales with large N as $R_N \sim N^\nu$, where ν depends on number of dimensions d as:

$$\nu \begin{cases} = 1, & d = 1 \\ = 3/4, & d = 2 \\ \approx 3/5, & d = 3 \\ = 1/2, & d \geq 4 \end{cases} \tag{5}$$

In 1 dimension the constraint gives straight-line polymer, in 4 or higher dimensions the constraint does not constrain polymer configurations.

2 General theory

We now proceed to the general theory of random walks with identically distributed correlated steps. For simplicity, we will assume that mean of the single step PDF is 0, and that variance of the single step PDF σ^2 is finite. Position $\vec{X}_N$ of the walker after N steps of individual displacements $\Delta\vec{x}_i$ is given by (1). The problem is to find $\vec{X}_N$.

Covariance between two random variables x_1 and x_2 is defined as:

$$\text{cov}(x_1, x_2) = \langle (x_1 - \langle x_1 \rangle)(x_2 - \langle x_2 \rangle) \rangle. \tag{6}$$

Correlation coefficient between two random variables x_1 and x_2 is defined as:

$$\rho = \frac{\text{cov}(x_1, x_2)}{\sigma_1 \sigma_2}, \tag{7}$$

where σ_1, σ_2 are variances of x_1 and x_2 respectively. It can be shown that $-1 \leq \rho \leq 1$ and that $\rho = 1$ for $x_2 = x_1$ and $\rho = -1$ for $x_2 = -x_1$.

With mean of PDF of each step equal to 0, mean of $\vec{X}_N$ is also 0:

$$\langle \vec{X}_N \rangle = \langle \sum_{n=1}^{N} \Delta\vec{x}_n \rangle = \sum_{n=1}^{N} \langle \Delta\vec{x}_n \rangle = \vec{0}. \tag{8}$$

The question we are going to be concerned with is how $\langle \vec{X}_N^2 \rangle$ scales with N. $\langle \vec{X}_N^2 \rangle$ can be determined from (1):

$$\langle \vec{X}_N^2 \rangle = \sum_{n=1}^{N} \sum_{m=1}^{N} \langle \Delta\vec{x}_n \cdot \Delta\vec{x}_m \rangle \tag{9}$$

Correlation matrix is defined as:

$$C_{n,m} = \langle \Delta\vec{x}_n \cdot \Delta\vec{x}_m \rangle \tag{10}$$

Assuming translational invariance in time (stationary process): $C_{n,m} = C(|m - n|)$, and (9) can be rewritten as:

$$\langle \vec{X}_N^2 \rangle = \sum_{n=1}^{N} \sum_{m=1}^{N} C(|m - n|) \tag{11}$$

This sum has N^2 terms; we group terms with $|m - n| = n' \neq 0$ and notice that number of such terms is $2(N - n')$: number of terms with $m - n = n'$ is easy to obtain by visualizing number of integer positions of rod of length $m - n = n'$ on a closed interval $[1; N]$; the factor of 2 comes from the modulus. Then, noticing that the number of terms with $n = m$ is N, and that $C(0) = \langle \Delta\vec{x}_i^2 \rangle = \sigma^2$, we obtain:

$$\langle \vec{X}_N^2 \rangle = N\sigma^2 + 2 \sum_{n'=1}^{N-1} C(n')(N - n') = N\sigma^2 + 2 \sum_{n'=1}^{N} C(n')(N - n'). \tag{12}$$

In the last equality we included a term with $n' = N$ in the sum since this term is equal to 0.

In the continuum limit $N = t/\tau$, $\tau \to 0$, $N \to \infty$. Correlation matrix of displacements $C(n')$ in this limit corresponds to velocity correlation function $\langle \vec{v}(0) \cdot \vec{v}(t') \rangle$, through

$$\langle \vec{v}(0) \cdot \vec{v}(t') \rangle = \langle \frac{\Delta \vec{x}_m}{\tau} \frac{\Delta \vec{x}_{m+n'}}{\tau} \rangle = \frac{C(n')}{\tau^2}, \qquad t' = n'\tau. \tag{13}$$

Noticing that $t = N\tau$, $t' = n'\tau$ and introducing $D_0 = \frac{\sigma^2}{2\tau}$, we can rewrite (12) as

$$\langle \vec{X}_N^2 \rangle = 2\tau N \cdot \frac{\sigma^2}{2\tau} + 2 \sum_{t'=\tau, 2\tau, \ldots}^{t} \frac{C(n')}{\tau^2} (t - t')\tau \tag{14}$$

$$= 2tD_0 + 2 \int_0^t \langle \vec{v}(0) \cdot \vec{v}(t') \rangle (t - t') dt, \qquad \tau \to 0. \tag{15}$$

In the limit $t \to \infty$ we expect $\langle \vec{X}_N^2 \rangle$ to scale as $\langle \vec{X}_N^2 \rangle \sim 2Dt$, and therefore $D = \frac{1}{2} \frac{d}{dt} \langle \vec{X}_N^2 \rangle$, and

$$D = \lim_{t \to \infty} \frac{1}{2} \frac{d}{dt} \langle X_N^2 \rangle = \lim_{t \to \infty} [D_0 + \int_0^t \langle \vec{v}(0) \cdot \vec{v}(t') \rangle dt'] \tag{16}$$

When the correlation time is much bigger than the time step τ, the first term can be neglected to yield Green-Kubo formula:

$$D = \int_0^\infty \langle \vec{v}(0) \cdot \vec{v}(t') \rangle dt', \tag{17}$$

i.e. integral of the velocity correlation function gives diffusion constant.

Breakdown of CLT (breakdown of diffusive scaling). Essentially, correlation controls whether diffusion is normal or not both in the discrete and the continuum cases, through value of D:

$$\text{Continuum case:} \qquad D = \int_0^\infty \langle \vec{v}(0) \cdot \vec{v}(t') \rangle dt' \tag{18}$$

$$\text{Discrete case:} \qquad D = \sum_{n'=1}^{\infty} C(n') \tag{19}$$

The following cases can be distinguished:

- If D is finite and non-zero, diffusion is normal: $\langle X_N^2 \rangle \sim 2Dt$ or $\langle X_N^2 \rangle \sim N$;
- If $D \to \infty$, diffusion is "superdiffusion", $\langle X_N^2 \rangle \sim N^\nu$, $1 < \nu \leq 2$;
- If $D \to 0$, diffusion is "subdiffusion", with $\langle X_N^2 \rangle \sim N^\nu$, $1 \leq \nu < 1$.

3 Example: exponentially decaying correlation

Let's consider a generic example of exponentially decaying in "time" correlation:

$$\langle \Delta \vec{x}_{n+1} \cdot \Delta \vec{x}_n \rangle = \rho\sigma^2, \qquad -1 < \rho < 1. \tag{20}$$

Then,

$$C(n) = \sigma^2 \rho^n. \tag{21}$$

Introducing decorrelation time $n_c = -2/\log\rho$:

$$C(n) = \sigma^2 e^{-2n/n_c} \tag{22}$$

It is now clear that correlation between steps exponentially decays with "time" (or number of steps) between the steps. A characteristic "time" (number of steps) after which correlation vanishes is n_c. In polymers it determines effective number of consecutive monomers with the same orientation (or number of "straight bonds" between bends). Later it will become clear that such polymers can be well approximated by random walk with N/n_c independent (uncorrelated) steps with step size n_c.

Dividing both sides of (12) by σ^2:

$$\begin{aligned}
\frac{\langle \vec{X}_n^2\rangle}{\sigma^2} &= N + 2\sum_{n=1}^{N-1}\rho^n(N-n) &(23)\\
&= -N + 2\sum_{n=0}^{N-1}\rho^n(N-n) &(24)\\
&= -N + 2N\sum_{n=0}^{N-1}\rho^n - 2\sum_{n=0}^{N-1}n\rho^n &(25)
\end{aligned}$$

The first sum in (25) is the geometric series:

$$S_N = \sum_{n=0}^{N-1}\rho^n = \frac{1-\rho^N}{1-\rho} \tag{26}$$

The second sum in (25) can be evaluated by differentiating (26) with respect to ρ:

$$\frac{dS_N}{d\rho} = \sum_{n=0}^{N-1} n\rho^{n-1} = \frac{1}{\rho}\sum_{n=0}^{N-1} n\rho^n \tag{27}$$

Therefore,

$$\begin{aligned}
\sum_{n=0}^{N-1} n\rho^n &= \rho\frac{dS_N}{d\rho} = \rho\frac{d}{d\rho}\left(\frac{1-\rho^N}{1-\rho}\right) &(28)\\
&= \rho\frac{(1-\rho)(-N\rho^{N-1}) + (1-\rho^N)}{(1-\rho)^2} &(29)
\end{aligned}$$

Substituting (26) and (29) in (25):

$$\begin{aligned}
\frac{\langle \vec{X}_n^2\rangle}{\sigma^2} &= -N + 2N\frac{1-\rho^N}{1-\rho} + 2\frac{N\rho^N}{1-\rho} - 2\frac{\rho(1-\rho^N)}{(1-\rho)^2} &(30)\\
&= \frac{1+\rho}{1-\rho}N - 2\frac{\rho(1-\rho^N)}{(1-\rho)^2}, &(31)
\end{aligned}$$

or,

$$\boxed{\frac{\langle \vec{X}_n^2\rangle}{N\sigma^2} = \frac{1+\rho}{1-\rho} - \frac{2}{N}\frac{\rho(1-\rho^N)}{(1-\rho)^2}.} \tag{32}$$

The first term in this formula is known, depending on a problem, as diffusion or noise term, the second term is known as advection, or ballistic, or signal term. This second term goes to 0 as $N \to \infty$, and the diffusion asymptotically follows

$$\langle \vec{X}_n^2 \rangle \sim 2DN\tau \tag{33}$$

with the diffusion coefficient D given by ($D_0 = \frac{\sigma^2}{2\tau}$)

$$\boxed{\frac{D}{D_0} = \frac{1+\rho}{1-\rho}.} \tag{34}$$

At small N the advection/ballistic/signal term dominates, but eventually diffusion/noise term wins.

It can be seen that the diffusion coefficient D is a monotonically increasing function of ρ, $D = 0$ when $\rho = -1$ and $D \to \infty$ when $\rho \to 1$. Now we will take a look at the ballistic-diffusion transition by considering limit $\rho \to 1$. Let $\rho = 1 - \epsilon$, $\epsilon \to +0$. Then

$$n_c = -\frac{2}{\log \rho} \sim \frac{2}{\epsilon}, \tag{35}$$

$$\frac{1+\rho}{1-\rho} \sim \frac{2}{\epsilon} = n_c, \qquad \frac{2}{N}\frac{\rho(1-\rho^N)}{(1-\rho)^2} \sim -\frac{n_c^2}{2N}\left(e^{-\frac{2N}{n_c}} - 1\right), \tag{36}$$

and (32) takes the form:

$$\frac{\langle \vec{X}_n^2 \rangle}{N\sigma^2} = n_c + \frac{n_c^2}{2N}\left(e^{-\frac{2N}{n_c}} - 1\right). \tag{37}$$

Introducing scaling variables $\tilde{N} = \frac{N}{n_c}$, $\tilde{X_N} = \frac{X_N}{n_c\sigma}$, we get the scaling function:

$$\boxed{\langle \tilde{X}_N^2 \rangle = \tilde{N} + \frac{1}{2}\left(e^{-2\tilde{N}} - 1\right), \qquad \rho \to 1.} \tag{38}$$

At $\tilde{N} \ll 1$ we are in the ballistic regime with slope of ($\log(\langle \tilde{X}_N^2 \rangle^{1/2})$ vs $\log \tilde{N}$) of 1, at $\tilde{N} \gg 1$ we have diffusive regime with the slope of 2 (Fig. 1, courtesy of Jaehyuk Choi, lect. 13, course 18.325, 2001).

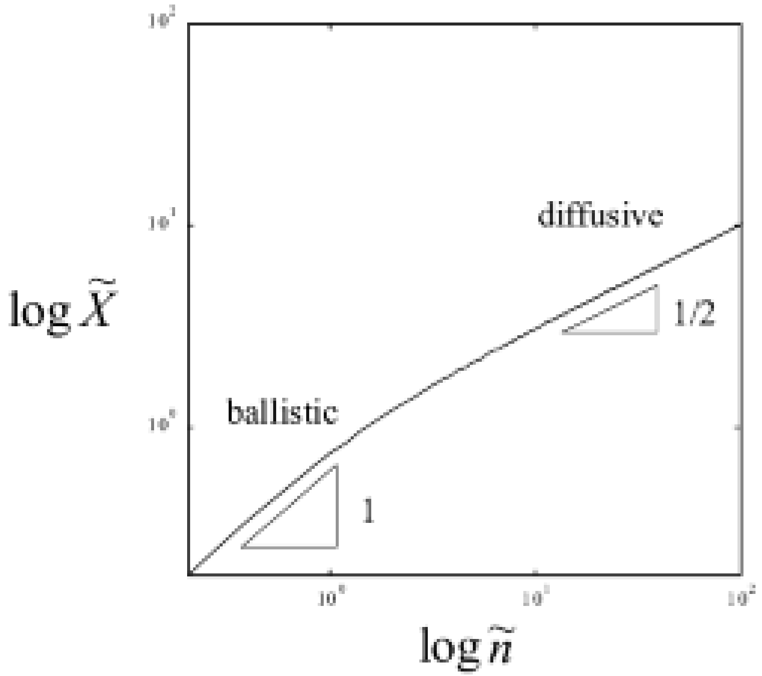

Figure 1: Ballistic-diffusive transition.